Future Space Applications of Compound Semi-conductor X-ray Detectors

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On the Development of Compound Semi-conductor Thallium Bromide Detectors for Astrophysics

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Future Space Applications of Compound Semiconductor X-ray Detectors

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Abstract

Detectors based on compound semiconductors have now reached a level of maturity, where they can be considered for use in a variety of space-based applications involving X-ray imaging optics. The possible range of space applications is reviewed and the key future requirements of these detectors discussed. These X-ray detectors will play a major role in future astrophysics and planetary missions. Recent results on the agency's X-ray detector research & development program into such materials as TlBr, epitaxial GaAs and CdZnTe are presented.

Keywords: X-ray detector, astrophysics, X-ray optics, compound semiconductors

1. Introduction

In this paper we describe the future use of compound semiconductor X-ray detector arrays for space research. X-ray spectroscopy has represented a key tool for space research from its very early days. Indeed X-astronomy has developed into a major field of astrophysics since the discovery of the first extra-solar X-ray source in 1962 [1]. Remote sensing of solar-system bodies lacking an atmosphere through the use of fluorescence spectroscopy with the sun used as the input energy source is also a rapidly developing field which owed its inception to the early Apollo flights of the 1970's [2]. Both these very different topics have in the past relied heavily on gas based detectors, such as proportional counters, while current missions have migrated into silicon based semiconductor technology. Indeed many current astrophysics missions such as XMM (ESA) utilize sophisticated X-ray CCD's having close to Fano limited resolution [3].

The European Space Agency (ESA) has for a number of years been developing a range of compound semiconductors (CS) for potential application in its future planetary and astrophysics missions. Table I shows some of the principal relevant properties of CS materials under study compared to silicon.

Table I : Some of the important detector related properties of materials compared to silicon which are under development as X-ray detectors at ESA

Material	Silicon	CdZnTe	GaAs	TlBr
Average Z	14	48.5	32	58
Density ρ (g cm ⁻³)	2.33	5.9	5.32	7.56
Band gap Δ @ RT(eV)	1.11	1.5-2.2	1.43	2.7
Pair creation energy ϵ (eV)	3.7	4.5	4.27	6.5
Fano Factor F	0.085	0.08	0.18	0.2
Electron mobility μ_e @ 300 K (cm ² V ⁻¹ s ⁻¹)	1500	1350	8000	6
Electron lifetime τ_e (s)	3 10 ⁻³	10 ⁻⁶	10 ⁻⁸	2.5 10 ⁻⁶
Electron mobility-lifetime product $\mu_e\tau_e$ (cm ² V ⁻¹)	4.5	1.35 10 ⁻³	8 10 ⁻⁵	1.5 10 ⁻⁵
Hole mobility μ_h @ 300 K (cm ² V ⁻¹ s ⁻¹)	600	120	400	?
Hole lifetime τ_h (s)	3 10 ⁻³	5 10 ⁻⁸	10 ⁻⁷	?
Hole mobility-lifetime product $\mu_h\tau_h$ (cm ² V ⁻¹)	1.8	6 10 ⁻⁶	4 10 ⁻⁵	2 10 ⁻⁵

2. Rationale

2.1 X-ray Optics

Future developments in astrophysics and planetary remote sensing will require the development of sophisticated X-ray imaging systems. Sensitive instruments will only be developed if the technology relating to X-ray optics progresses together with that of the X-ray detectors used at their focus. The basic principles for the focussing of X-rays using grazing incidence mirrors is of course well established and an example system is illustrated in figure 1. Here a nested Wolter-I optic is shown, although other designs such as Kirkpatrick-Baez are also possible depending on the application [4]. Note that for most astrophysical applications the Wolter-I (or its variants) is the design of choice. From figure 1 the geometrical area of such a telescope is simply: $A_{Geo} = \sum 2\pi r_o^i L_p^i \tan(\alpha^i)$, where the index i simply refers to the shell number in the nest. The effective area after reflection by on-axis X-rays can then be written as: $A(E) = \sum A_{Geo}^i R(\alpha^i, E)^2$, where E is the energy of the incident photon and R is the reflectivity off one of the surfaces (paraboloid or hyperboloid), which depends on the Fresnel equations and the complex index of refraction ($n = 1 - \delta - i\beta$). The critical angle is then: $\alpha_c \sim (2\delta)^{0.5}$, where δ is the real part of the refractive index. Finally the focal length, a key parameter effecting the spacecraft design is written: $f = r_o^i / \tan(4\alpha^i)$.

From these equations defining the nested Wolter -I system we see that a large aperture (large r_i) cannot be effective as the photon energy increases without a decrease in the graze angle α_i from the critical angle α_c . As α_i decreases then the focal length must increase. For photons with energy of 1 & 10 keV the critical angles for a gold reflecting surface are 3.5° and $\sim 0.5^\circ$ respectively.

Figure 1: A schematic of a nested Wolter-I X-ray telescope which focuses X-rays to the focal point. A pixelated CS detector is assumed at the focus.

Closed surfaces of revolution such as those used in the Chandra (USA) and XMM missions lead ultimately to a limit on the overall aperture size ($\sim 1m$) and hence on the achievable effective area. Indeed XMM (ESA) and ASCA (J) have attempted to a limited extent to break out of this area constraint by having more than one co-aligned telescope (three in the case of XMM). This of course only makes effective use of the aperture at low energies for a fixed focal length, and of course leads to a proliferation of focal plane instruments [5]. Future astrophysics missions such as XEUS: The X-ray Early Universe Spectroscopy mission currently under study by

ESA will require many tens of square meters of collecting area implying aperture diameters for the single telescope of over 10 m [6]. This aperture can be achieved by segmenting the mirror aperture into "petals". Figure 2 (a) shows such a petal. Each paraboloid-hyperboloid is formed as a single piece (as in XMM) but now as an open surface, the radius of which depends on the section of the aperture occupied by the petal. The degree of nesting and the overall geometry of the petal depend on the plate manufacturing process. For XEUS electroformed nickel plates as shown in figure 2(b) are currently base-lined.

The critical parameter governing the effective collecting area is the focal length, which has in the past been effectively dictated by the size of the spacecraft, which in turn is generally controlled by the physical size of the launcher. Despite the development of extendable optical benches – c.f. ASCA there are limits to such an approach (currently ~ 10 m). XEUS has also broken this constraint by effectively introducing two spacecraft: one containing the mirrors and the second containing the focal plane detector array. In the case of XEUS the focal length (i.e. the separation between the two spacecraft) is 50 m, being limited now only by the attitude and orbit control system. Future missions may well increase this baseline significantly. With such focal lengths, now for the first time, the graze angles are sufficiently small to provide considerable collecting area in a truly imaging-focussing instrument at medium - higher X-ray energies. For example at 20 keV the XEUS collecting area is ~1000 cm² all of which can be used to focus a source of harder X-rays onto an imaging solid state detector.

(b)

Figure 2: (a) Schematic of a XEUS mirror petal, (b) examples of XEUS electroformed nickel plates.

The very small graze angles required to efficiently reflect higher energy X-rays (typically - 4° at 30 keV) implies that most of the conventional Wolter-I optics aperture shown in Figure 1 is blocked by the thickness of the reflecting surfaces (shells or plates). This means a massive optics with a low efficiency unless a route can be established to produce very thin reflecting surfaces. The technology utilized in the production of micro-channel plates offers this possibility [7]. This approach should allow thin walled channels, which have a geometry such that a tandem pair of plates can efficiently bring the X-rays to a single focus. Figure 3 (a)

illustrates schematically the principle while figure 3 (b) shows an electron microscope image of a prototype plate prior to undergoing medium energy X-ray tests at ESA. Each focussing square pore channel is $\sim 10 \times 10 \mu\text{m}^2$.

Of course not only could this approach be a step forward in the X-ray performance at higher energies, but such plates could be used at much lower energies allowing a far lighter optics to be constructed. Such an approach would have major applications in planetary remote sensing as well as possibly giving rise to ground-based spin-offs such as fluorescent microscopy, medical imaging and X-ray lithography. Note for the remote sensing of solar system bodies without atmospheres such as Mercury, the Moon or asteroids from a spacecraft in orbit around such an object this implies that spacecraft resources such as mass, power and volume all must all be conserved.

Figure 3 (a): A schematic of a MCP optics system, which would allow a significant collecting aperture at hard X-ray energies while reducing the overall mirror mass. **(b)** An electron microscope image of a few channels from a prototype plate.

2.2 Astrophysical X-ray Spectroscopy

Any plasma at a temperature above 10^6 K radiates the bulk of its energy as X-rays from collisional excitation line emission and thermal bremsstrahlung continuum processes. At low temperatures ($< 10^7$ K) the bulk of this photon emission is in the form of emission lines radiated in the soft X-ray band (< 2 keV) while at much higher temperatures ($> 10^8$ K) the continuum emission processes dominate. This only arises as a result of the fact that since at higher temperatures the majority of ions with a low atomic number are completely stripped of their electrons while the remaining ions are hydrogenic or helium-like species such elements as sulfur and iron.

Medium resolution x-ray spectroscopy using compound semiconductors can provides the ability to determine the electron temperatures and density, the relative abundance of the elements as well as establishing the degree of thermal and ionization equilibrium, possibly without recourse to the rather low operating temperatures required by some silicon based devices. The measurement of the intensity of the hydrogenic and helium like lines from the same element is an important ion temperature indicator. Table II summarizes the key hydrogenic & helium -like transition energies from some of the most abundant elements expected to be present in an astrophysical plasma, together with the Fano limited resolution at these energies for a number of semiconductors. Clearly a CSS such as CZT or GaAs, provided they can achieve a Fano limited resolution, should be capable of resolving these key transitions. To illustrate this point figure 4 shows the response of a number of semiconductor detectors to the X-ray flux expected to be radiated from an optically thin plasma having a temperature 10^7 K. In this example solar abundances and ionization equilibrium were assumed and for clarity the continuum emission, the spectral shape of which provides a measure of the thermal bremsstrahlung electron temperature, has been suppressed. The majority of lines are rather well resolved with such a CZT detector enabling, through the measurement of the relative intensity of the lines the temperature and relative abundances to be determined. Note the intensity ratio of lines from different ions of the same element, together with line centroids, allows one to deduce not only the ion temperature but also either the degree of ionization equilibrium or possibly distance to the object, through the determination of the red-shift z .

Table II : The principle line transitions of the most abundant lines together with the Fano limited resolution of various semiconductors

Element	E(H)	E(He)	E(H)-E(He)	$\Delta E(\text{Si})$	$\Delta E(\text{CZT})$	$\Delta E(\text{GaAs})$
Iron	6702	6963	260	108	116	169
Sulfur	2460	2621	160	66	70	102
Silicon	1864	2006	140	57	61	89
Oxygen	574	653	80	32	34	49

$\Delta E(\text{eV})$ the Fano limited resolution at the helium like line energy based on the Fano factors of Table I.
E(H) is the energy centroid in eV of the hydrogenic line and E(He) refers to the helium-like line.

Figure 4: The simulated response of a Fano limited CZT semiconductor detector in the range 2-10 keV to the radiation emitted from a hot plasma with a temperature of 10^7 K.

At higher energies the electron-thermal bremsstrahlung process gives rise to a smooth featureless continuum which requires an accurate measurement at high energies (>10 keV) to really establish the shape and thus plasma electron temperature. Other continuum emission mechanisms at these energies, which dominate in many cosmic X-ray sources, are non-thermal such as synchrotron radiation and various Compton emission processes. The spectra of a number of accreting X-ray pulsars do however contain line features between 10-50 keV due to electron cyclotron transitions in the high magnetic field ($> 10^{12}$ G) of the neutron star. The energy of the fundamental cyclotron harmonic E_{cyc} is related to the neutron star magnetic field strength in units of 10^{12} G (B_{12}) by the relation $E_{\text{cyc}} = 11.6 B_{12} (1+z)^{-1}$ keV, where z is the gravitational redshift. Thus the observation of cyclotron features in the hard X-ray spectra of accreting X-ray sources gives a direct measurement of the magnetic field. In general a cyclotron feature will be an absorption feature since the photon-electron scattering is very large in the magnetized plasma.

Finally electron positron annihilation lines at 512 keV possibly in distant extra-galactic sources which may be redshifted to lower energies as $(1+z)$ are expected in a number of accretion fed X-ray sources.

2.3 Planetary Remote Sensing X-ray Fluorescent Spectroscopy

Future exploration of the solar system will involve the geo-chemical mapping of many solar system bodies in order to better understand the process of planet formation and the evolution of the system since its birth. Airless bodies such as those discussed above and also including the moons of the great planets are best mapped through X-ray fluorescent spectroscopy from a co-orbiting spacecraft [8].

The basic principles of X-ray mapping are clear. Solar X-rays are absorbed directly by the surface elements and produce characteristic K- and L-shell lines from the surface material. The relative strengths of these lines provide the data from which to determine indirectly the surface geology. The solar flux is sufficiently intense to be absorbed in the first few tens of microns of the surface producing not only the fluorescent lines from light elements (C, O, Na, Mg, Al, Si) but also from the heavier elements (Ca, Ti and Fe). Figure 5 illustrates the response expected from a surface of the type C1 carbonaceous chondrite meteorite if observed by an imaging telescope coupled to a CSS detector made from CdZnTe. The detector was assumed to have near Fano limited resolution. This simulation includes the abundances of the elements appropriate for this type of meteorite as well as the fluorescent yield and branching ratios of the various elements. It does not for simplicity include the interaction of the solar flux with the surface or the scattering and radiation transport within the surface material.

Even with these gross simplifications it is clear that a near Fano limited CZT detector operating close to room temperature would be a valuable tool with which to probe the surface chemistry of some solar system solid bodies.

Figure 5 : The simulated emission spectrum from a carbonaceous chondrite meteorite after illumination by X-rays as observed by a Fano limited CZT. Note the log scale for the counts received. Clearly the fluorescent emission from some of the lower energy K lines will be seriously modified by radiation transport through the surface layer.

3. Compound Semiconductors

While current astrophysics missions such as ASCA/Chandra/AXAF or SAX use silicon CCD's or gas detectors future missions under development (e.g. XEUS) will make use of low temperature cryogenic detectors as well as silicon based devices. Note ASTRO-E due for launch in 2000 will also contain a cryogenic detector. However the higher energy response (> 10 keV), important for future developments in high energy astrophysics may well be best addressed through the use of CSS based pixilated arrays [9]. In addition it must be noted that current missions for planetary fluorescent studies only utilize silicon and are rather basic in design e.g. no X-ray focusing optics. Previous missions were based on non-imaging proportional counters with rather poor energy resolution compared to solid state detectors.

3.1 High Energy (10-200 keV) X-ray Spectroscopy with TlBr Detectors

Thallium bromide (TlBr) has a high average atomic number ($Tl = 81$ and $Br = 35$) and density (c.f. Table I) such that it could become an efficient room temperature compound detector for hard X-ray energies (10 - 200 keV). ESA has embarked on a development program for TlBr detectors with a view to producing pixilated arrays capable of being used together with micro-channel plate based optics (figure 3) to image and detect hard X-rays from cosmic sources. Figure 6 illustrates the mean penetration depth and Fano limited resolution of TlBr as a function of X-ray photon energy. As can be seen, the efficiency would be still as high as 10 % for a TlBr crystal with a thickness of 1 mm even at 1 MeV. While such a thick crystal has been produced it is clear that the upper energy threshold will be driven by the capabilities of the optics rather than the TlBr crystal. The inset of Figure 6 shows the response of such a 0.8 mm thick TlBr 2.7x2.7 mm monolithic detector to a high energy ^{241}Am radioactive source. While the Fano limited resolution ($\Delta E_{\text{Fano}} \sim 380$ eV at 20 keV) has not yet

been achieved, an important mechanism causing the resolution degradation has been determined to be due to leakage currents in the vicinity of the contacts, rather than simply material related issues such as crystal purity or crystal dislocations introducing traps. This can be seen from the $\mu\tau$ product shown in Table 1. At ~ 20 keV the measured resolution $\Delta E_{\text{Measured}} \sim 2.1$ keV while the system noise (including the major contribution from the leakage current is $\Delta E_{\text{Noise}} \sim 1.6$ keV, leading to an intrinsic detector resolution of $\Delta E_{\text{Intrinsic}} \sim 1.3$ keV, which is within a factor of 3.5 from the Fano limited resolution.

Figure 6 . The mean penetration depth and Fano limited resolution of TIBr as a function of X-ray photon energy. The inset shows the measured spectrum from 0.8 mm thick TIBr crystal when illuminated by Np – L lines from a Am^{241} radioactive source. The operating temperature was -2°C .

3.2 Medium Energy (2-100 keV) X-ray Spectroscopy with Epitaxial GaAs Detectors

Pixilated detectors based on epitaxial gallium arsenide would appear to be very effective in covering the X-ray energy range 2-100 keV yet operating close to room temperature (-35°C). If leakage currents can be reduced further then the energy range might be extended below 1 keV. This would allow GaAs detectors to fulfil the dual roles as a detector for low & medium energy spectroscopy. Figure 7 shows the mean penetration depth and Fano limited resolution of GaAs as a function of X-ray photon energy. The efficiency would be still as high as 10 % for GaAs based detector with a thickness of $400 \mu\text{m}$ at 100 keV. Such a thick epitaxial GaAs has been produced, indeed we are currently working with 1 mm thick epitaxial GaAs having an efficiency of $\sim 30\%$ at 100 keV. The inset of Figure 7 shows the response of a $40 \mu\text{m}$ thick GaAs detector to lower energy X-rays from a monochromatic synchrotron source (3-5 keV). Currently energies as low as 2 keV are detectable. Note the equivalent system noise includes a significant contribution from the leakage current and electronics which in this case contains additional noise due to EMC pick-up from the synchrotron beam environment. The measured resolution at 4 keV is $\Delta E_{\text{Measured}} \sim 670$ eV. While at these lower X-ray energies the Fano limited resolution (130 eV at 4 keV) is still a long way off, resolution degradations caused by issues of crystal purity (based on the measured $\mu\tau$ products shown in Table I) are effectively solved and now leakage currents in the vicinity of the contacts are the main source of resolution degradation.

Figure 7: The mean penetration depth and Fano limited resolution of GaAs as a function of X- ray photon energy. The inset shows the measured spectrum from 40 μm thick epitaxial GaAs when illuminated by monochromatic soft X-rays from a synchrotron source having energies of 3, 4 and 5 keV. The operating temperature was -35°C .

At higher X-ray energies the situation is rather encouraging. Figure 8 shows the response of a 40 μm thick epitaxial GaAs detector to 20 keV monochromatic X-rays from a synchrotron source. Up to 5 harmonics (P3-P8) and their escape peaks (E3-E8) are clearly resolved. The inset shows in detail the energy-loss spectrum around the primary photo-peak P1 and its escape peaks E1. Note the Ga & As $K\alpha$ escapes lines are resolvable. At ~ 60 keV the measured resolution $\Delta E_{\text{Measured}} \sim 1.1$ keV while the system noise (including the major contribution from the leakage current) is $\Delta E_{\text{Noise}} \sim 0.7$ keV leading to an intrinsic detector resolution of $\Delta E_{\text{Intrinsic}} \sim 0.85$ keV. This is within a factor of 1.7 of the Fano limited resolution of $\Delta E_{\text{Fano}} \sim 0.5$ keV. Such a detector would be rather effective in detecting the cyclotron lines expected from accreting neutron stars.

Figure 8: The measured spectrum from 40 μm thick epitaxial GaAs when illuminated by monochromatic 20 keV X-rays from a synchrotron source. The operating temperature was -40°C .

The quality of the epitaxial GaAs material is now such that a serious development of large format pixilated imaging detectors can be considered.

3.3 Low Energy X-ray Line Spectroscopy (1-10 keV) with CdZnTe

Detectors based on CdZnTe are generally considered as potential detectors for hard x-ray spectroscopy. However they, together with the GaAs detectors discussed above, may also have an application at low energies, particularly in the field of planetary fluorescent spectroscopy where operating temperature may become a real issue. Figure 9 shows the mean penetration depth and Fano limited resolution of this material as a function of x-ray photon energy. The hard X-ray capability is clear however such detectors may well also have a serious capability at soft X-ray wavelengths. Figure 9 also therefore shows (insert) the response of a CZT detector to various low energy monochromatic x-ray photons from a synchrotron source. The measured resolution was $\Delta E_{\text{Measured}} \sim 400\text{ eV}$ at 1.7 keV while the system noise was $\Delta E_{\text{Noise}} \sim 350\text{ eV}$ leading to an intrinsic detector resolution of $\Delta E_{\text{Intrinsic}} \sim 190\text{ eV}$. Again the major contribution to the system noise was the leakage current considered to be associated with the contacts. This means that this material is within a factor of ~ 3 of the Fano limited resolution of $\Delta E_{\text{Fano}} \sim 60\text{ eV}$.

Figure 9: The mean penetration depth and Fano limited resolution of CZT as a function of X- ray photon energy. The inset shows the measured low energy spectrum from a 5x5x2mm thick crystal when illuminated by monochromatic x-rays from a synchrotron source. Three energies, 1.2, 1.5 & 2 keV, are shown. The operating temperature was -30°C .

4. Conclusions

The development of compound semiconductors for X-ray astrophysics and planetary fluorescent X-ray spectroscopy has now reached a state of development where serious applications of pixilated detectors combined with major developments in X-ray optics can now be considered. We have summarized here the key results relating to TlBr, GaAs and CdZnTe based detectors. Providing the leakage currents can be further reduced such materials offer a serious competitive advantage over silicon for specific applications.

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